

1H-Imidazole-2-sulfonic acid  
53744-47-1 | DTXSID40601515

Model Performance

|       |      |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.95            | 0.69 | 0.95           | 0.65 | 0.96       | 0.68 |

Model Results

Predicted value: 7.84

Global applicability domain: Outside

Local applicability domain index: 2.55e-01

Confidence level: 4.22e-01

Nearest Neighbors from the Training Set

|  |   |  |
|--|---|--|
| <div>Image not found</div> <div>4-Hydroxybenzoic acid</div> <div>Measured: 8.08</div> <div>Predicted: 7.78</div> | <div>Image not found</div> <div>Salicylic acid</div> <div>Measured: 7.44</div> <div>Predicted: 7.60</div> | <div>Image not found</div> <div>Methylparaben</div> <div>Measured: 8.57</div> <div>Predicted: 7.06</div> |
| <div>Image not found</div> <div>1-Octanol</div> <div>Measured: 6.03</div> <div>Predicted: 5.95</div>             | <div>Image not found</div> <div>Phenacetin</div> <div>Measured: 9.59</div> <div>Predicted: 9.23</div>     |  |